

On the Simulation of Extended TDHF Theory *

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Abstract

A novel method is presented for implementation of the extended mean-field theory incorporating two-body collisions. At a given time, stochastic imaginary time propagation of occupied states are used to generate a convenient basis. The quantal collision terms, including memory effects, is then computed by a backward mean-field propagation of these single-particle states. The method is illustrated in an exactly solvable model. Whereas the usual TDHF fails to reproduce the long time evolution, a good agreement is found between the extended TDHF and the exact solution.

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1 Introduction

Mean-field approximation is often employed to study static and dynamical properties of many-body systems in different branches of physics including atomic physics, condensed matter and nuclear physics [1]. The complex quantal many-body dynamics is reduced to an effective one-body problem, in which particles move under an effective self-consistent mean-field potential without experiencing correlations. Such an approach, which is usually referred to as Hartree-Fock (HF) in static limit and Time-Dependent Hartree-Fock (TDHF) in dynamics, is best suited at low energies at which binary collisions have little effects on dynamics since scattering into unoccupied states is severely inhibited due to Pauli blocking. The HF and TDHF models have been very successful in describing many static and dynamical properties in nuclear physics at low energies [2, 3, 4, 5]. In heavy-ion collisions around Fermi energy, dynamical evolution exhibits strong dissipation and fluctuation properties. Mean-field alone is inadequate to describe the collision dynamics at these energies, and it is necessary to improve the one-body description beyond the mean-field approximation by incorporating binary collisions due to short range correlations into the equation of motion. This model is usually referred to as the extended TDHF (ETDHF)[6, 7, 8, 9]. A large amount of work has been done on the formal development of the ETDHF, however, due to the numerical complexity often linked with conceptual problems, the applications of the theory on realistic situations remain a difficult problem, and only a few approximate quantal calculations exists so far [10, 11, 12, 13]. Most of the applications of this theory have been carried out in semi-classical approximation, known as the Boltzmann-Uehling-Uhlenbeck (BUU) model [14]. It has been very successful for understanding a variety of features associated with nuclear collisions at intermediate energies, including collective flow and particle production. It is generally taken for granted that the test particle simulation of the BUU model provides a good approximation for the average dynamics for small quantal systems that we face with in heavy ion-collisions. The actual test of the semi-classical models should be made by comparing the test particle simulations with quantum transport calculations. Such a comparisons has been made in the mean-field approximation in a recent work [20, 21], and demonstrated that the expansion dynamics exhibits quantum effects which persists up to rather high temperature $T \approx 5MeV$. Furthermore, the quantal features may play even more important role during the disassembly phase of the reaction. Therefore, it is off great interest to

develop quantal transport descriptions of heavy-ion dynamics.

In this paper, we propose a practical method for obtaining numerical solutions of the ETDHF theory in its quantal version, and illustrate the method in an exactly solvable model[15]. We study a fermionic case but the method can be applied to treat bosonic or even mixed systems.

2 Extended Mean-Field Theory

The basic idea of one body approaches is to project the dynamics onto the single-particle density matrix $\rho(t)$. In the ETDHF theory the evolution of $\rho(t)$ is determined by a transport equation,

$$i\hbar \frac{\partial \rho}{\partial t} - [h[\rho], \rho] = K[\rho]. \quad (1)$$

The left hand side describes the evolution under the effective mean-field Hamiltonian which may be related to the energy functional $E[\rho]$ as $h[\rho] = \partial E[\rho]/\partial \rho$ [16], and the right hand side represents a quantal binary collision term [17]. It is convenient to express the collision term in the natural representation $|\psi_\lambda(t)\rangle$ which diagonalizes the single-particle density matrix

$$\rho(t) = \sum |\psi_\lambda(t)\rangle n_\lambda(t) \langle \psi_\lambda(t)|. \quad (2)$$

Then, the matrix elements of the collision term are given by [12]

$$\langle \psi_\lambda(t) | K[\rho] | \psi_{\lambda'}(t) \rangle = -\frac{i}{\hbar} \left(F_{\lambda, \lambda'}(t) + F_{\lambda', \lambda}^*(t) \right) \quad (3)$$

with

$$F_{\lambda, \lambda'}(t) = \frac{1}{2} \int_{t_0}^t dt' \sum \langle \lambda \delta' | v_{12} | \alpha \beta \rangle_A |_t \langle \alpha' \beta' | v_{12} | \gamma \delta \rangle_A |_{t'} \\ (\rho_{\gamma \lambda'} \rho_{\delta \delta'} \bar{\rho}_{\alpha \alpha'} \bar{\rho}_{\beta \beta'} - \rho_{\alpha \alpha'} \rho_{\beta \beta'} \bar{\rho}_{\gamma \lambda'} \bar{\rho}_{\delta \delta'}) |_{t'} \quad (4)$$

where $\bar{\rho}_{\lambda \lambda'}(t) = \delta_{\lambda \lambda'} - \rho_{\lambda \lambda'}(t)$ and v_{12} denotes an effective residual interaction. The matrix elements of the residual interaction are given as

$$\langle \alpha \beta | v_{12} | \lambda \delta \rangle_A |_{t'} = \langle \bar{\psi}_\alpha(t') \bar{\psi}_\beta(t') | v_{12} | \bar{\psi}_\lambda(t') \bar{\psi}_\delta(t') \rangle_A \quad (5)$$

where $\langle \cdot \rangle_A$ denotes the antisymmetrized matrix element, and the states $|\bar{\psi}_\lambda(t')\rangle$ are obtained by backward propagation of the natural states from time t to

t' by the mean-field propagator, $|\bar{\psi}_\lambda(t')\rangle = U^\dagger(t, t') |\psi_\lambda(t)\rangle$, where the mean-field propagator is given by

$$U(t, t') = T \exp \left(-\frac{i}{\hbar} \int_{t'}^t h[\rho(s)] ds \right) \quad (6)$$

with T as the time-ordering operator. In the collision term (4), $\rho_{\lambda\lambda'}(t') = \langle \bar{\psi}_\lambda(t') | \rho(t') | \bar{\psi}_{\lambda'}(t') \rangle$ denotes the elements of density matrix at time t' in the basis of the backward propagated states and it can be expressed as

$$\rho_{\lambda\lambda'}(t') = \sum \langle \bar{\psi}_\lambda(t') | \psi_\alpha(t') \rangle n_\alpha(t') \langle \psi_\alpha(t') | \bar{\psi}_{\lambda'}(t') \rangle \quad (7)$$

where $n_\alpha(t')$ denotes the occupation number of the natural state $|\psi_\alpha(t')\rangle$.

The collision term involves usually two characteristic times: the correlation time τ_{cor} of the matrix elements of the residual interactions and the relaxation time τ_{rel} of the occupation numbers[18]. The expression of the collision term is valid when the correlation time is much smaller than the relaxation time, $\tau_{cor} \ll \tau_{rel}$, which is usually referred to as the weak coupling limit. The time integration over the past history is evaluated over a time interval $t - t_0$ which should be sufficiently larger than the correlation time τ_{cor} . In this case, since during the correlation time, the natural states deviate only slightly from the states propagated with the mean-field, we may approximate the overlap as $\langle \bar{\psi}_\lambda(t') | \psi_{\lambda'}(t') \rangle \simeq \delta_{\lambda\lambda'}$, and as a result, the collision term takes a simple form

$$F_{\lambda,\lambda'}(t) \simeq \frac{1}{2} \int_{t_0}^t dt' \sum \langle \lambda \delta | v_{12} | \alpha \beta \rangle_A |_t \langle \alpha \beta | v_{12} | \lambda' \delta \rangle_A |_{t'} \quad (8)$$

$$(n_{\lambda'} n_\delta \bar{n}_\alpha \bar{n}_\beta - n_\alpha n_\beta \bar{n}_\lambda \bar{n}_\delta) |_{t'}.$$

Furthermore, in accordance with the weak-coupling limit this expression may be further simplified by neglecting the evolution of the occupation numbers during the correlation time by taking them as $n_\lambda(t') \simeq n_\lambda(t)$.

3 Numerical method

For the purpose of numerical iteration, it is convenient to transform the transport eq.(1) into an integral form. Given the density matrix at a time t in terms of the occupied states $|\psi_\lambda(t)\rangle$ and associated occupation numbers

$n_\lambda(t)$, its evolution during a time interval Δt may be expressed according to

$$\begin{aligned} \rho(t + \Delta t) = & U(t + \Delta t, t) \rho(t) U(t, t + \Delta t) \\ & - \frac{i}{\hbar} \int_t^{t+\Delta t} ds U(t + \Delta t, s) K(s) U(s, t + \Delta t) \end{aligned} \quad (9)$$

where the first term represents the pure mean-field evolution and the second term is the perturbation caused by the collision term during the time interval Δt . Single-particle states $|\bar{\psi}_\lambda(t + \Delta t)\rangle$ obtained by propagating the natural states from time t to $t + \Delta t$ according to (6), provide a useful basis to calculate density matrix over short time intervals. In this representation, the elements of the density matrix at time $t + \Delta t$ may approximately be given by

$$\rho_{\lambda\lambda'}(t + \Delta t) \simeq n_\lambda(t) \delta_{\lambda\lambda'} - \frac{1}{\hbar^2} \int_t^{t+\Delta t} ds [F_{\lambda\lambda'}(s) + F_{\lambda'\lambda}^*(s)] \quad (10)$$

where $F_{\lambda\lambda'}(s)$ is computed according to Eq. (4) or its approximate form (8) assuming that over the time interval Δt the natural states can be approximated by $|\bar{\psi}_\lambda(s)\rangle$. At time $t + \Delta t$ the new natural states $|\psi_\lambda(t + \Delta t)\rangle$ and their occupation numbers $n_\lambda(t + \Delta t)$ are determined by diagonalizing the occupation matrix $\rho_{\lambda\lambda'}(t + \Delta t)$. Then, the iteration is continued into the next time step in a similar manner. The time interval Δt of the numerical iteration can be taken larger than the typical numerical time-step of the mean-field evolution, but it should be smaller than the correlation time to insure at most one collision takes place during the interval. When the collision term in eq.(9) is a small perturbation, a full diagonalization of the density matrix is not needed, and the new states and the changes in the occupation numbers can be calculated using perturbation theory. However, to insure numerical stability, it is always possible to include higher orders. The occupation numbers are determined by the diagonal elements of (11) which can be transformed into a generalized master equation,

$$\frac{d}{dt} n_\lambda(t) = \int_{t_0}^t dt' \{ \bar{n}_\lambda(t') \mathcal{W}_\lambda^+(t, t') - n_\lambda(t') \mathcal{W}_\lambda^-(t, t') \} \quad (11)$$

where the gain \mathcal{W}_λ^+ and loss \mathcal{W}_λ^- kernels are given by

$$\mathcal{W}_\lambda^+(t, t') = \frac{1}{\hbar^2} \sum Re \{ \langle \lambda \delta | v_{12} | \alpha \beta \rangle_A |_t \langle \alpha \beta | v_{12} | \lambda \delta \rangle_A |_{t'} \} n_\alpha(t') n_\beta(t') \bar{n}_\delta(t') \quad (12)$$

and

$$\mathcal{W}_\lambda^-(t, t') = \frac{1}{\hbar^2} \sum Re \{ \langle \lambda \delta | v_{12} | \alpha \beta \rangle_A |_t \langle \alpha \beta | v_{12} | \lambda \delta \rangle_A |_{t'} \} \bar{n}_\alpha(t') \bar{n}_\beta(t') n_\delta(t') \quad (13)$$

According to perturbation theory, when the states are non-degenerate, the new natural states at time $t + \Delta t$ may be expressed as,

$$|\psi_\lambda(t + \Delta t)\rangle = |\bar{\psi}_\lambda(t + \Delta t)\rangle - \frac{1}{\hbar^2} \sum_{\lambda' \neq \lambda} \frac{1}{n_\lambda(t) - n_{\lambda'}(t)} |\bar{\psi}_{\lambda'}(t + \Delta t)\rangle \int_t^{t+\Delta t} ds \{F_{\lambda\lambda'}(s) + F_{\lambda'\lambda}^*(s)\}. \quad (14)$$

This expression emphasizes importance of the non-diagonal terms in the collision kernel which insure a proper transformation of the occupied states. With the diagonalization procedure the collision term itself decides the structure of the important single-particle states to be populated. For the application presented in this paper, we have used a direct diagonalisation technics instead of a perturbative approach to define the waves functions.

The collision term $F_{\lambda\lambda'}(t)$ involves, in addition to the occupied single-particle states $|\psi_\lambda^{occu}(t)\rangle$ which are known, a complete set of unoccupied states. Specification of the most relevant set of intermediate states in a reasonable manner has been the major difficulty in the implementation of the ETDHF theory. Some effort has been made to generate the unoccupied states by the TDHF evolution in the same manner as the occupied states [12]. Since it is difficult to guess from the beginning of the reaction, the relevant unoccupied states, which are strongly coupled with occupied states during a binary collision, may not be generated by a TDHF evolution. Moreover, the unoccupied states generated in this manner may escape to continuum before having a chance to participate in a possible binary collision.

In this article, we propose an algorithm to construct the relevant unoccupied states at each stage of the iteration directly from the occupied states by employing a stochastic imaginary time propagator method as follows. At the beginning of each time step Δt , a series of states is generated by repeated application of the imaginary time propagator $U_\beta^{(n)} = \exp[-\beta(h[\rho] + \delta h^{(n)})]$ on the occupied states $U_\beta^{(n)} |\psi_\lambda^{(n-1)}(t)\rangle = |\psi_\lambda^{(n)}(t)\rangle$ with $|\psi_\lambda^{(0)}(t)\rangle = |\psi_\lambda^{occu}(t)\rangle$. The series of states obtained by application of the propagator $\exp(-\beta h[\rho])$ generate a restricted subspace which has the same symmetry properties as the occupied states. On the other hand relevant unoccupied states may have different symmetry properties, and therefore, may lie outside of this subspace. In order to ensure symmetry breaking and to perform a faster sampling of the relevant configuration[19], a stochastic part $\delta h^{(n)}$ is added to the the mean-field Hamiltonian at each application of the propagator $U_\beta^{(n)}$.

In the case of open systems, the continuum may also be treated by adding a density-dependent constraining field into $\delta h^{(n)}$. These series of linearly independent states together with the occupied states are orthonormalized using a Schmidt procedure after each application of $U_\beta^{(n)}$. In this manner, it is possible to construct a suitable subspace of properly orthonormalized single-particle basis $\{|\psi_\lambda(t)\rangle\}$ including both occupied $|\psi_\lambda^{occu}(t)\rangle$ and unoccupied states $|\psi_\lambda^{unoc}(t)\rangle$. The subspace of the unoccupied states may be truncated further by diagonalizing the mean-field Hamiltonian $h[\rho(t)]$ in this subspace and by removing the states with energies larger than a maximum amount. The high frequency components of the occupied states have only a minor effect in the collision term, since they damp out very quickly in time and because of the time integration in eq. (4) and (6). The construction with the help of the imaginary time propagator diminishes the high frequency components, and at the same time, it generates a space of the unoccupied states in terms of linear combinations of predominantly the low frequency components of each occupied states. In practice, for an approximate treatment of the collision term, it may be sufficient to generate the relevant unoccupied states by a few applications of U_β on the occupied states. The sensitivity of the results on the approximate treatment can be checked by enlarging the subspace of unoccupied states. The unoccupied and occupied states are then evolved backward in time using the mean-field propagator order to properly take into account the past history in the collision term. We should note that, the high frequency components of the basis may become important for increasing available energy, and the method may depend on the structure of the residual interaction. Therefore, the method should be tested carefully before applications to nuclear collision dynamics around Fermi energy.

4 First Application

We illustrate the method in a one dimensional model problem of two identical fermions coupled to a total spin projection $m_S = 0$, i.e. one with spin up and one with spin down, which are moving in an external anharmonic potential and are interacting via a short range two-body force. The Hamiltonian of the system is given by

$$H = \sum_{i=1,2} \left(\frac{p_i^2}{2m} + \frac{k}{2}(x_i - x_0)^2 + \frac{k'}{4}(x_i - x_0)^4 \right) + v_{12} \quad (15)$$

with $k = -0.04$ MeV/fm², $k' = 0.08$ MeV/fm⁴, $x_0 = 9.3$ fm. In this schematic model, we avoid the problem of construction of a G-matrix by employing a simple force without a hard core. This force mimics the effective interaction usually employed in mean-field approaches, and also simplifies the discussion on the role of the collision term. We should note that the same effective interaction should be used in both the collision term and in the mean-field part of the ETDHF equation. The two-body interaction is taken as

$$v_{12} = v_0 \exp\left[-\frac{(x_1 - x_2)^2}{2\sigma^2}\right] \quad (16)$$

with $v_0 = -4$ MeV and $\sigma = 2$ fm. We consider the system initially prepared in a constrained equilibrium state at a temperature $T=5$ MeV. The initial two-particle density matrix is, therefore, represented by

$$D_{12}(t=0) = \sum_i |\Psi_i\rangle \frac{\exp[-E_i/T]}{Z} \langle \Psi_i| \quad (17)$$

where the initial two-particle states are determined by solving a constrained Schroedinger equation, $(H - \lambda Q) |\Psi_i\rangle = E_i |\Psi_i\rangle$ with Q as a one-body constraining field, which is taken as $Q = \sum_i \lambda(x_i)(x_i - x_0)^2$ with $\lambda = -0.24$ MeV/fm² for $x_i > x_0$ and $\lambda = -0.12$ MeV/fm² for $x_i < x_0$. We follow the exact Liouville von Neumann evolution of the two-particle density matrix $D_{12}(t)$ by evolving each two-particle states $|\Psi_i(t)\rangle$ with the time-dependent Schroedinger equation. We compare the exact evolution of the single-particle density matrix $\rho_1(t) = \text{tr}_2 D_{12}(t)$ with the approximate evolutions obtained in the TDHF and the ETDHF descriptions, starting with the same initial conditions. In the simulations, the numerical time-step is taken as 0.5 fm/c whereas the collision term is evaluated in larger time intervals of $\Delta t = 6$ fm/c. In the calculation, we employ a harmonic potential with a stochastic strength for δh and two iterations of the imaginary time propagator appeared to be sufficient to generate the relevant unoccupied states. Figure 1 shows the time evolution of the local single-particle density $\rho(x, t)$ as a function of the position x . Until about 100 fm/c, the TDHF calculation shown by dashed lines provides a good approximation for the exact evolution indicated by dotted lines, but is not able to reproduce it for larger times. On the other hand, the ETDHF results indicated by solid lines are in good agreement with the exact evolution even at large times. Figure 2 illustrates the evolution of the expectation value of the center of mass coordinate $\langle X(t) \rangle$, as a

function of time. Also for this observable, the ETDHF result (solid line) follows closely the exact evolution (dotted line), whereas the TDHF calculation (dashed line) deviates from the exact evolution at large times. Time evolution of the occupation numbers of time-dependent single-particle states are plotted in figure 3. The ETDHF calculations shown by dashed lines are very close to the exact evolution indicated by open circles, which are obtained by a direct diagonalization of $\rho_1(t) = tr_2 D_{12}(t)$. In the pure TDHF approach, the occupation numbers remain constant and equal to their initial values.

5 conclusion

Even though the formal development of the ETDHF theory was available for some time, only a few applications in some simplified model problems have been carried out so far. The major problem of the numerical implementation originates from the difficulties for a realistic treatment of the collision term in a suitable representation. In order to overcome this difficulty, we propose a possible method in which the most important unoccupied states, those strongly coupled with the occupied states through the collision term, are calculated dynamically at each time step and then evolved backward in time using the mean-field propagator in order to treat the past history in the collision term. We illustrate the method in an exactly solvable one-dimensional system of two-particles, and find that the description of the one-body density matrix in the ETDHF is in good agreement with the exact evolution. In realistic applications to nuclear collision dynamics, the method may be implemented using the existing TDHF codes since it requires only standard calculation of the residual interaction matrix elements and usual mean-field propagation in real and imaginary time. In these applications, the computational effort is not small, and may require a factor of about 20-100 more computation time than the corresponding TDHF simulation, but becomes manageable with high computational power of present day computer technology. In fact, a first step in this direction has been recently taken [22]. In this work, collective vibrations at finite temperature have been investigated in the small amplitude limit of the ETDHF theory, including the collisional term. Such a calculation requires the computation of many matrix elements as in the full ETDHF description. The work for simulations of the full theory for large amplitude collective motion is currently in progress. We should also note that, the ETDHF theory is relevant to not only nuclear dynam-

ics. Therefore, the proposed method may provide a useful tool for describing dissipation and fluctuation phenomena in other quantal systems.

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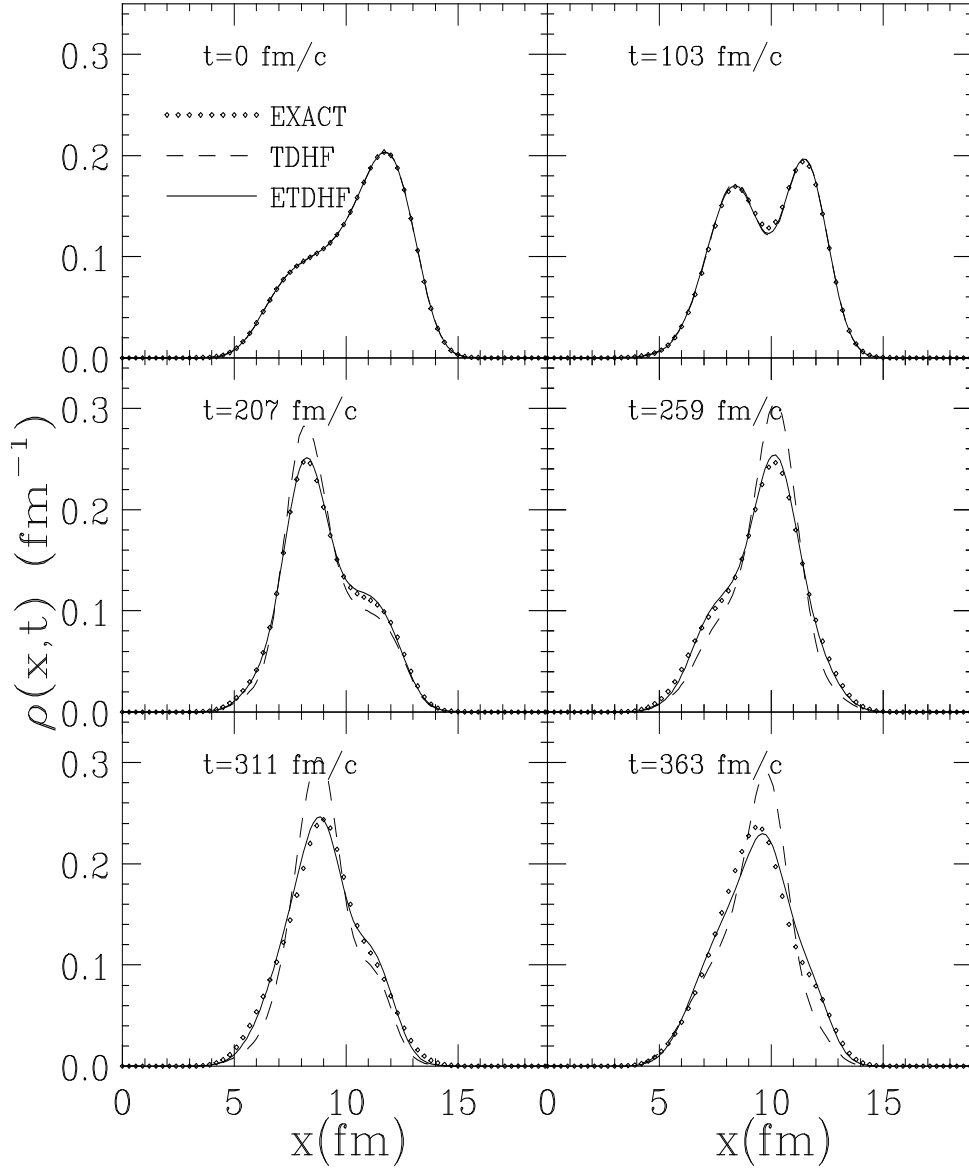


Figure 1: Evolution of the local density. The exact calculations, the TDHF and the ETDHF results are shown by circles, dashed lines and solid lines, respectively.

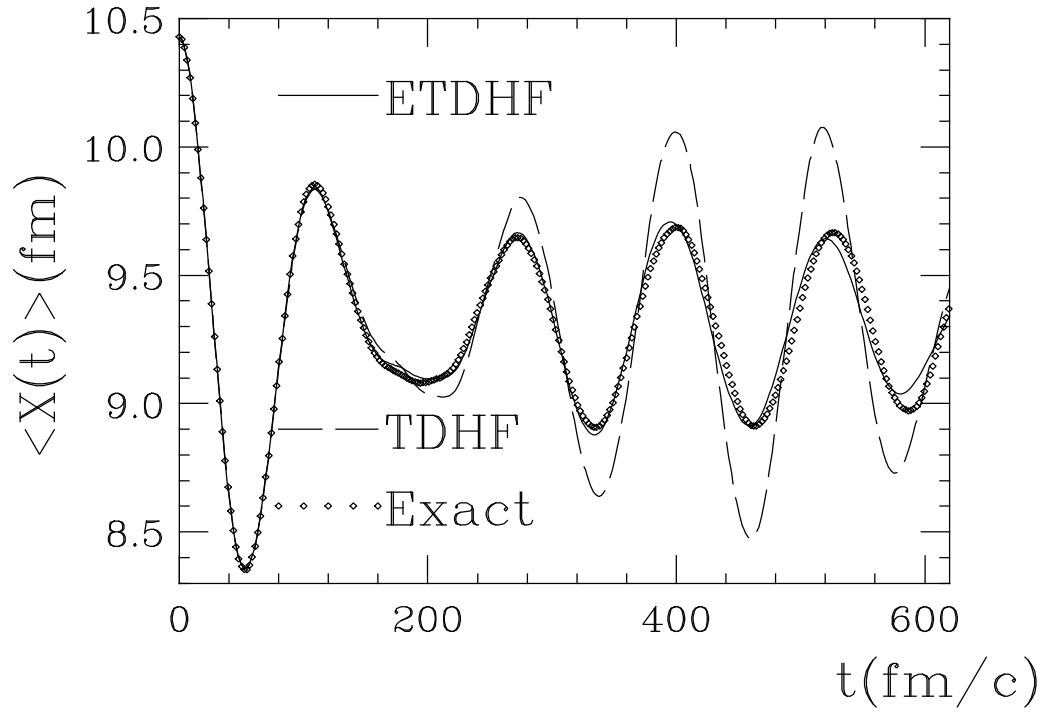


Figure 2: Expectation value of the center of mass as a function of time. The exact calculation, the TDHF and the ETDHF results are shown by circles, dashed line and solid line, respectively.

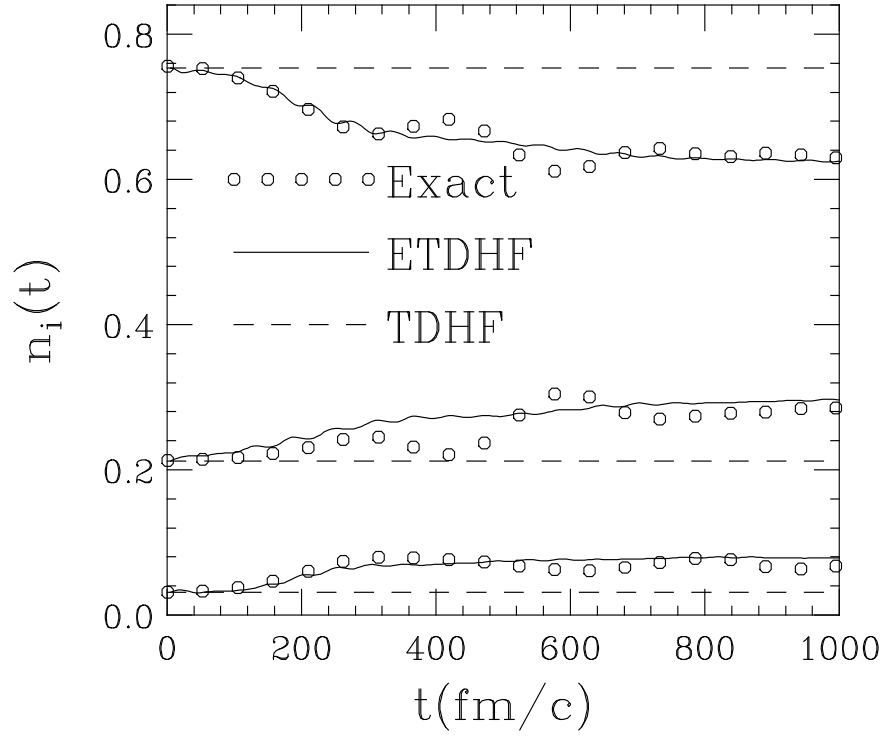


Figure 3: Occupation numbers as a function of time. The exact calculations, the TDHF and the ETDHF results are shown respectively by circles, dashed and solid lines.